

Green's function technique for a two-electrode mesoscopic system under bias

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We present a Green's function technique for studying the nonlinear conductance of a nanocontact system with two electrodes at different chemical potentials. The retarded Green's function for a single-impurity Anderson model with two reservoirs is obtained in terms of a 5×5 matrix in which the effect of bias is contained. A complete set of basis vectors for the single-impurity Anderson model has been provided before formulating the Green's function. Finally, we present a self-consistent method to fix the undetermined quantities existing in the matrix elements for the retarded Green's function.

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I. INTRODUCTION

The single-particle Green's function is a basic tool for studying the correlation effects in many-body systems. However, calculation of this function in the case of a strongly correlated system is not usually successful because such a calculation generally requires nonperturbative treatment. Moreover, the possibility of a successful calculation becomes even less when the system is under steady-state nonequilibrium (SSN) conditions. Recently, some mesoscopic systems having nanocontact features have attracted considerable interest. Such systems include a quantum point contact [1–4], a single electron transistor with a quantum dot [5–8], and magnetic atom adsorbed on a metallic surface [9–12]. Experimentalists measure the dI/dV in these systems for a given V ; I and V denote the current and the bias, respectively. Because of the bias, resonant tunneling occurs unidirectionally in the ground state. This unidirectional tunneling causes the system to be out of the linear response regime. Therefore, nonlinear conductances observed for the abovementioned systems may not be explained by a linear response theory. The purpose of this study is to provide a Green's function technique that is suitable for studying the nonlinear conductance of a mesoscopic system operating under bias.

A well-known formula for a steady current passing through a small interacting region that is connected to charge reservoirs having different chemical potentials was proposed more than a decade ago [13, 14]. This formula is given by

$$I = -\frac{e}{\hbar} \int \frac{d\omega}{2\pi} \frac{\Gamma^L(\omega)\Gamma^R(\omega)}{\Gamma^L(\omega) + \Gamma^R(\omega)} [f_L(\omega) - f_R(\omega)] \times \text{Im}G_{dd\sigma}^+(\omega; V) \quad (1)$$

for proportional lead functions, i.e., $\Gamma^L(\omega) \propto \Gamma^R(\omega) = 2\pi \sum_{\sigma} \rho_{\sigma}^R(\omega) |V_{kd}^R|^2$, where σ indicates spin, L and R denote the left and right reservoirs, respectively, $\rho_{\sigma}^R(\omega)$ is the density of states of the right metallic reservoir without inter-electron interaction, and V_{kd}^R is the strength of hybridization between the state d of interacting region and the state k of the right reservoir. Further, $f_L(\omega)$ in

Eq. (1) denotes the Fermi distribution function of the left reservoir. Since unidirectional tunneling at ground state is a unique characteristic of the SSN, the effect of bias must be appeared explicitly in the retarded Green's function in Eq. (1). However, to the best of our knowledge the steady-state Green's function for the quantum impurity system has not been obtained yet.

The purpose of this study is to present a method for determining the steady-state retarded Green's function appearing in Eq. (1). To realize this method, we adopt the retarded Green's function expressed in resolvent operator form in the Heisenberg picture [15]; this function is given by

$$iG_{ij\sigma}^+(z) = \langle c_{i\sigma} | (z\mathbf{I} + i\mathbf{L})^{-1} | c_{j\sigma} \rangle, \quad (2)$$

where $z = -i\omega + \eta$ and $c_{i\sigma}$ indicates annihilation of a fermion with spin σ at a state i . The symbols \mathbf{I} and \mathbf{L} in Eq. (2) denote the identity operator and the Liouville operator, respectively. The latter is defined by $\mathbf{L}\hat{O} = [\mathcal{H}, \hat{O}] = \mathcal{H}\hat{O} - \hat{O}\mathcal{H}$, where \mathcal{H} and \hat{O} are the Hamiltonian operator and an arbitrary operator, respectively. Although we are familiar with the resolvent form in the Schrödinger picture,

$$G_{ij}^+(\omega) = \langle \phi_i | (\omega + i\eta - \mathcal{H})^{-1} | \phi_j \rangle, \quad (3)$$

where ϕ_j is an eigenstate of \mathcal{H} , we employ Eq. (2) in this study because a dynamical approach using operators is more appropriate for describing electron hopping under steady-state conditions.

This paper is composed as follows: In section II, we present a systematic method to determine a complete set of basis vectors for calculating the retarded Green's function given in Eq. (2). A single-impurity Anderson model with one- and two-reservoir is studied as an example. In section III, we express the retarded Green's function for a two-reservoir system under bias in terms of a finite-dimensional matrix and discuss the physical meanings of the matrix elements. We present a self-consistent method to determine unknown quantities in section IV and finally give conclusions in section V.

II. DETERMINING COMPLETE SET OF BASIS VECTORS

The first step in the calculation of the retarded Green's function in resolvent form, Eq. (2), is ensuring a complete set of basis vectors. It should be noted that the resolvent form does not provide information about the orthogonal basis vectors. Therefore, the Lanczos algorithm [16, 17] in the Schrödinger picture and the projection operator technique [18, 19] in the Heisenberg picture are used to obtain static and dynamic orthogonal basis vectors, respectively. However, employing the Gram-Schmidt orthogonalization procedure to obtain orthogonal basis vectors for a nontrivial system causes significant complications. Hence, we propose a new and simpler technique for obtaining the basis vectors.

The retarded Green's function in Eq. (2) can be obtained by calculating the matrix inverse $(\mathbf{M}^{-1})_{11}$, where \mathbf{M} is composed of the elements

$$\mathbf{M}_{ij} = z\delta_{ij} - \langle i\hat{\mathbf{L}}\hat{e}_j | \hat{e}_i \rangle = z\delta_{ij} + \langle \hat{e}_j | i\hat{\mathbf{L}}\hat{e}_i \rangle, \quad (4)$$

once a complete basis set, $\{\hat{e}_\ell | \ell = 1, \dots, \infty\}$, spanning the Liouville space is given. We select $\hat{e}_1 = c_{d\sigma}$ to obtain $G_{dd\sigma}^+(\omega)$. The inner product in Eq. (4) is defined by $\langle \hat{e}_k | \hat{e}_\ell \rangle \equiv \langle \{\hat{e}_k, \hat{e}_\ell^\dagger\} \rangle$, where the angular and curly brackets denote the statistical average and anticommutator, respectively. We now present a systematic method for determining the basis vectors. For this purpose, expressing the Green's function operator in a diagonal matrix as

$$iG_{ij\sigma}^+(z) = (\langle \hat{A} | \langle \hat{B} |) \begin{pmatrix} \hat{G}_A & 0 \\ 0 & \hat{G}_B \end{pmatrix} \begin{pmatrix} |\hat{A}\rangle \\ |\hat{B}\rangle \end{pmatrix} \quad (5)$$

is the most crucial step. Once this form is achieved, the Liouville space of $G_{ij\sigma}^+(z)$ will be spanned completely by the linearly independent components of vectors $|\hat{A}\rangle$ and $|\hat{B}\rangle$. To obtain the form in Eq. (5), we expand the Green's function operator $\hat{G} = [z\mathbf{I} + i(\mathbf{L}_I + \mathbf{L}_C)]^{-1}$, where \mathbf{L}_I and \mathbf{L}_C respectively represent the Liouville operators for the isolated part \mathcal{H}_I and the connecting part \mathcal{H}_C of the Hamiltonian; The operator is expanded in powers of \mathbf{L}_C using the operator identity $(\hat{A} + \hat{B})^{-1} = \hat{A}^{-1} - \hat{A}^{-1}\hat{B}(\hat{A} + \hat{B})^{-1}$, where $\hat{A} = z\mathbf{I} + i\mathbf{L}_I$ and $\hat{B} = i\mathbf{L}_C$. Then, after resumming the expansion, the retarded Green's function can be expressed as follows:

$$\begin{aligned} iG_{ij\sigma}^+(z) &= \langle c_{i\sigma} | \hat{G}_I | c_{j\sigma} \rangle - \langle c_{i\sigma} | \hat{G}_I | i\mathbf{L}_C \hat{G}_I | c_{j\sigma} \rangle \\ &+ \langle c_{i\sigma} | \hat{G}_I | i\mathbf{L}_C | \hat{G} | i\mathbf{L}_C \hat{G}_I | c_{j\sigma} \rangle, \end{aligned} \quad (6)$$

where $\hat{G}_I \equiv (z\mathbf{I} + i\mathbf{L}_I)^{-1}$. Equation (6) can be written in the matrix form as

$$iG_{ij\sigma}^+(z) = (\langle c_{i\sigma} | \langle \Phi_i |) \mathbf{G} (|c_{j\sigma}\rangle | \Phi_j \rangle)^T, \quad (7)$$

where $\mathbf{G} = \begin{pmatrix} \hat{G}_I & -\hat{G}_I \\ 0 & \hat{G} \end{pmatrix}$, $|\Phi_j\rangle = |i\mathbf{L}_C \hat{G}_I c_{j\sigma}\rangle$, and the superscript T denotes the transpose. Using the lin-

ear transformation $\mathbf{U} = \begin{pmatrix} I & -\hat{G}_{LT} \\ 0 & I \end{pmatrix}$, where $\hat{G}_{LT} = \hat{G}_I / [\hat{G} - \hat{G}_I]$, one can diagonalize \mathbf{G} . Equation (7) is then modified as

$$iG_{ij\sigma}^+(z) = (\langle \tilde{c}_{i\sigma} | \langle \Phi_i |) \mathbf{G}_D (|\tilde{c}_{j\sigma}\rangle | \Phi_j \rangle)^T, \quad (8)$$

where $\mathbf{G}_D = \begin{pmatrix} \hat{G}_I & 0 \\ 0 & \hat{G} \end{pmatrix}$ and

$$\begin{aligned} |\tilde{c}_{j\sigma}\rangle &= |c_{j\sigma}\rangle + (\hat{G}_I - \hat{G})^{-1} \hat{G}_I |\Phi_j\rangle \\ &= |c_{j\sigma}\rangle + [\mathbf{L}_C^{-1}(-iz\mathbf{I} + \mathbf{L})\Phi_j]. \end{aligned} \quad (9)$$

Equation (8) is the desired form and the linearly independent components of vectors $|\tilde{c}_{j\sigma}\rangle$ and $|\Phi_j\rangle$ completely span the Liouville space of $G_{ij\sigma}^+(\omega)$. In conclusion, the systematic method for collecting the basis vectors involves determining all linearly independent components comprising the vector $|\tilde{c}_{j\sigma}\rangle$ because $|\Phi_j\rangle$ is contained in this vector.

We will subsequently demonstrate the determination of the basis vectors by means of an example. We are interested in a mesoscopic system with a mediating Kondo atom between two metallic reservoirs. This system can be described by a single-impurity Anderson model with two metallic reservoirs, whose Hamiltonian is expressed as

$$\begin{aligned} \mathcal{H} &= \sum_{k,\sigma,\alpha=L,R} \epsilon_k c_{k\sigma}^{\alpha\dagger} c_{k\sigma}^\alpha + \sum_{\sigma} \epsilon_d c_{d\sigma}^\dagger c_{d\sigma} + U n_{d\uparrow} n_{d\downarrow} \\ &+ \sum_{k,\sigma,\alpha=L,R} (V_{kd} c_{d\sigma}^\dagger c_{k\sigma}^\alpha + V_{kd}^* c_{k\sigma}^{\alpha\dagger} c_{d\sigma}), \end{aligned}$$

where ϵ_k , ϵ_d , V_{kd} , and U indicate the energies of an electron of momentum k in lead, the level of a mediating atom, the hybridization between the atom and lead, and the on-site Coulomb repulsion at the atom, respectively. Because the two-reservoir Anderson model is a straightforward extension of the one-reservoir model, we consider a one-reservoir Anderson model as an example. Its isolated and coupled parts are given by

$$\mathcal{H}_I = \sum_{k,\sigma} \epsilon_k c_{k\sigma}^\dagger c_{k\sigma} + \sum_{\sigma} \epsilon_d c_{d\sigma}^\dagger c_{d\sigma} + U n_{d\uparrow} n_{d\downarrow}, \quad (10)$$

and

$$\mathcal{H}_C = \sum_{k,\sigma} (V_{kd} c_{d\sigma}^\dagger c_{k\sigma} + V_{kd}^* c_{k\sigma}^\dagger c_{d\sigma}). \quad (11)$$

We first demonstrate the calculation of $\Phi_d = i\mathbf{L}_C(\mathbf{I} + i\mathbf{L}_I)^{-1} c_{d\uparrow}$ and then of $|\tilde{c}_{d\sigma}\rangle$ for \mathcal{H}_I and \mathcal{H}_C above. It can be clearly observed that $(\mathbf{I} + i\mathbf{L}_I)^{-1} c_{d\uparrow}$ yields only two operators, $c_{d\uparrow}$ and $n_{d\downarrow} c_{d\uparrow}$. Applying \mathbf{L}_C to these operators changes the index $d(k)$ into $k(d)$ in fermion operators and $n_{d\downarrow}$ into $j_{d\downarrow}^-$. Therefore, the components of Φ_d are given by

$$\Phi_d = (c_{k\uparrow}, \quad n_{d\downarrow} c_{k\uparrow}, \quad j_{d\downarrow}^- c_{d\uparrow}), \quad (12)$$

where $k = 1, 2, \dots, \infty$ and

$$j_{d\downarrow}^- = i \sum_k (V_{kd} c_{d\downarrow}^\dagger c_{k\downarrow} - V_{kd}^* c_{k\downarrow}^\dagger c_{d\downarrow}). \quad (13)$$

We now focus on the vector $|\tilde{c}_{d\sigma}\rangle$ in Eq. (9). The operator $\mathbf{L}\Phi_d = [H, c_{k\uparrow}] + [H, n_{d\downarrow} c_{k\uparrow}] + [H, j_{d\downarrow}^- c_{d\uparrow}]$ yields $c_{d\uparrow}$ and $c_{k\uparrow}$ from the first commutator; $n_{d\downarrow} c_{d\uparrow}$, $n_{d\downarrow} c_{k\uparrow}$, and $j_{d\downarrow}^- c_{k\uparrow}$ from the second commutator; and $j_{d\downarrow}^- c_{d\uparrow}$, $j_{d\downarrow}^- c_{k\uparrow}$, $j_{d\downarrow}^+ c_{d\uparrow}$, $j_{d\downarrow}^- n_{d\downarrow} c_{d\uparrow}$, and $j_{d\downarrow}^+ n_{d\downarrow} c_{d\uparrow}$ from the third commutator, where

$$j_{d\downarrow}^+ = \sum_k (V_{kd} c_{d\downarrow}^\dagger c_{k\downarrow} + V_{kd}^* c_{k\downarrow}^\dagger c_{d\downarrow}). \quad (14)$$

The last operator $j_{d\downarrow}^+ n_{d\downarrow} c_{d\uparrow}$ is a vanishing one, and the operator $j_{d\downarrow}^- n_{d\downarrow} c_{d\uparrow}$ is dynamically equivalent to $j_{d\downarrow}^- c_{d\uparrow}$. Thus, the linearly independent components of $(\mathbf{I} + \mathbf{L})\Phi_d$ are classified into two groups, one involving $c_{k\uparrow}$ and the other involving $c_{d\uparrow}$. These components are

$$(\mathbf{I} + \mathbf{L})\Phi_d^k = (c_{k\uparrow}, \quad n_{d\downarrow} c_{k\uparrow}, \quad j_{d\downarrow}^- c_{k\uparrow}), \quad (15)$$

for $k = 1, 2, \dots, \infty$, and

$$(\mathbf{I} + \mathbf{L})\Phi_d^d = (c_{d\uparrow}, \quad n_{d\downarrow} c_{d\uparrow}, \quad j_{d\downarrow}^- c_{d\uparrow}, \quad j_{d\downarrow}^+ c_{d\uparrow}). \quad (16)$$

Finally, we apply \mathbf{L}_C^{-1} , which is equivalent to the repeated application of \mathbf{L}_C , to the operators in Eqs. (15) and (16). It can be clearly observed that the multiple application of \mathbf{L}_C to $c_{k\uparrow}$, $c_{d\uparrow}$, and $n_{d\uparrow}$ simply reproduces the existing operators and $j_{d\downarrow}^+ c_{k\uparrow}$. The remaining linearly independent operators arise from $\mathbf{L}_C^n j_{d\downarrow}^\mp$, where $n = 1, 2, \dots, \infty$. Thus, one may classify the basis vectors into two groups,

$$\text{Set of } c_{d\uparrow} = \{c_{d\uparrow}, \quad n_{d\downarrow} c_{d\uparrow}, \quad j_{d\downarrow}^- c_{d\uparrow}, \quad j_{d\downarrow}^+ c_{d\uparrow}, \\ (\mathbf{L}_C^n j_{d\downarrow}^\mp) c_{d\uparrow}, \quad (\mathbf{L}_C^n j_{d\downarrow}^\mp n_{d\downarrow}) c_{d\uparrow}\} \quad (17)$$

and

$$\text{Set of } c_{k\uparrow} = \{c_{k\uparrow}, \quad n_{d\downarrow} c_{k\uparrow}, \quad j_{d\downarrow}^- c_{k\uparrow}, \quad j_{d\downarrow}^+ c_{k\uparrow}, \\ (\mathbf{L}_C^n j_{d\downarrow}^\mp) c_{k\uparrow}\}. \quad (18)$$

The operators shown in Eqs. (17) and (18) describe all the possible linearly independent ways of annihilating an up-spin at site d in time t . In other words, these operators completely span the Liouville space of $c_{d\uparrow}(t)$.

It is important to identify the meaning of the basis vectors $(\mathbf{L}_C^n j_{d\downarrow}^\mp) c_{k\uparrow}$ and $(\mathbf{L}_C^n j_{d\downarrow}^\mp) c_{d\uparrow}$ for later discussion. Application of \mathbf{L}_C to $j_{d\downarrow}^\mp$ gives rise to

$$\mathbf{L}_C j_{d\downarrow}^- = -i \sum_l \sum_k (V_{ld} V_{kd}^* c_{l\downarrow}^\dagger c_{k\downarrow} + V_{kd} V_{ld}^* c_{k\downarrow}^\dagger c_{l\downarrow}) \\ + 2i \sum_k |V_{kd}|^2 c_{d\downarrow}^\dagger c_{d\downarrow}$$

and

$$\mathbf{L}_C j_{d\downarrow}^+ = \sum_l \sum_k V_{ld} V_{kd}^* c_{l\downarrow}^\dagger c_{k\downarrow} - \sum_l \sum_k V_{ld}^* V_{kd} c_{k\downarrow}^\dagger c_{l\downarrow}.$$

These operators represent a round trip of a down-spin electron between the mediating atom and electron reservoir. Therefore, $(\mathbf{L}_C^n j_{d\downarrow}^\mp)$ depicts n -time trip of a down-spin electron between the mediating atom and the reservoir without coming into contact with an up-spin electron at the mediating atom. This phenomenon rarely occurs in reality, and we neglect these basis vectors.

III. RETARDED GREEN'S FUNCTION FOR TWO-ELECTRODE SYSTEM

We identify the basis vectors that do not play an important role in describing the dynamics $c_{d\uparrow}(t)$ in the Kondo regime. We first consider the basis vector $n_{d\downarrow} c_{d\uparrow}$ in Eq. (17). Since $n_{d\downarrow}^2 = n_{d\downarrow}$, this basis vector describes the dynamical processes involving all higher orders of Coulomb interaction U . Therefore, in the Kondo regime, $n_{d\downarrow} c_{d\uparrow}$ must be eliminated. The operator $j_{d\downarrow}^- n_{d\downarrow} c_{d\uparrow}$ in Eq. (17) also represents the process that costs energy U or more. Therefore, we eliminate the basis vectors $(\mathbf{L}_C^n j_{d\downarrow}^- n_{d\downarrow}) c_{d\uparrow}$ in studying the Kondo regime. We further eliminate the basis vectors $(\mathbf{L}_C^n j_{d\downarrow}^\mp) c_{d\uparrow}$ because multiple round trip of an up-spin electron without coming into contact with a down-spin electron at the mediating atom are practically rare. These approximations are valid for describing the Kondo processes. Now, we discuss on the basis vectors combined with c_k shown in Eq. (18). These basis vectors contribute to constructing the self-energy. It is sufficient to choose c_k and $n_{d\downarrow} c_{k\uparrow}$ in Eq. (18) to construct the self-energy. The basis vectors $(\mathbf{L}_C^n j_{d\downarrow}^\mp) c_{k\uparrow}$ are eliminated by the same reason eliminating $(\mathbf{L}_C^n j_{d\downarrow}^\mp) c_{d\uparrow}$ in Eq. (17) and the contribution by $j_{d\downarrow}^\mp c_{k\uparrow}$ is much smaller than that by $n_{d\downarrow} c_{k\uparrow}$.

Finally, we obtain the reduced Liouville space constructed by the basis vectors

$$(c_{d\uparrow}, \quad j_{d\downarrow}^- c_{d\uparrow}, \quad j_{d\downarrow}^+ c_{d\uparrow}) \quad \text{and} \quad (c_{k\uparrow}, \quad n_{d\downarrow} c_{k\uparrow}),$$

where $k = 1, 2, \dots, \infty$ for describing the dynamics of the single-impurity Anderson model in the Kondo regime.

Since the resolvent form of $G_{dd\uparrow}^+(z)$ is given by the Laplace transform of the coefficient $a_1(t)$ in the expansion $c_{d\uparrow}(t) = \sum_{i=1}^\infty a_i(t) \hat{e}_i$, where $\hat{e}_1 = c_{d\uparrow}$, the equality $a_1(t) = G_{dd\uparrow}^+(t)$ must be obtained. This equality is valid when all the basis vectors except $c_{d\uparrow}$ are orthogonal to $c_{d\uparrow}$. This orthogonality condition is satisfied by introducing the expression $\delta \hat{A} = \hat{A} - \langle \hat{A} \rangle$ for the operators $n_{d\uparrow}$ and $j_{d\uparrow}^\mp$. Thus, we finally obtain the reduced Liouville space spanned by the basis vectors

$$(c_{d\uparrow}, \quad \delta j_{d\downarrow}^- c_{d\uparrow}, \quad \delta j_{d\downarrow}^+ c_{d\uparrow}) \quad \text{and} \quad (c_{k\uparrow}, \quad \delta n_{d\downarrow} c_{k\uparrow}),$$

where $k = 1, 2, \dots, \infty$, for the one-reservoir Anderson model in the Kondo regime. In practical calculations,

we use the normalized forms of the basis vectors. The basis vectors given above are the same as those used in the previous study [20], in which the basis vectors were obtained intuitively. The Liouville space for the two-reservoir Anderson model is a straightforward extension of that for the single-reservoir model. The basis vectors are given by

$$(c_{k\uparrow}^L, \delta n_{d\downarrow} c_{k\uparrow}^L), \text{ where } k = 1, 2, \dots, \infty; \text{ and}$$

$$(\delta j_{d\downarrow}^{+L} c_{d\uparrow}, \delta j_{d\downarrow}^{-L} c_{d\uparrow}, c_{d\uparrow}, \delta j_{d\downarrow}^{-R} c_{d\uparrow}, \delta j_{d\downarrow}^{+R} c_{d\uparrow}) \text{ and}$$

$$(\delta n_{d\downarrow} c_{k\uparrow}^R, c_{k\uparrow}^R), \text{ where } k = 1, 2, \dots, \infty,$$

where the superscripts L and R denote the left and right metallic leads, respectively. The matrix \mathbf{M} of Eq. (4) is expressed as

$$\mathbf{M} = \begin{pmatrix} \mathbf{M}_{LL} & \mathbf{M}_{dL} & \mathbf{0} \\ \mathbf{M}_{Ld} & \mathbf{M}_d & \mathbf{M}_{Rd} \\ \mathbf{0} & \mathbf{M}_{dR} & \mathbf{M}_{RR} \end{pmatrix}, \quad (19)$$

where \mathbf{M}_d is the 5×5 block that is constructed by the basis vectors

$$(\delta j_{d\downarrow}^{+L} c_{d\uparrow}, \delta j_{d\downarrow}^{-L} c_{d\uparrow}, c_{d\uparrow}, \delta j_{d\downarrow}^{-R} c_{d\uparrow}, \delta j_{d\downarrow}^{+R} c_{d\uparrow});$$

\mathbf{M}_{LL} , the $\infty \times \infty$ block constructed by the basis vectors $(c_{k\uparrow}^L, \delta n_{d\downarrow} c_{k\uparrow}^L)$, where $k = 1, 2, \dots, \infty$; and \mathbf{M}_{dL} , for example, a $5 \times \infty$ block constructed by the basis vectors given above.

The retarded Green's function $G_{dd\uparrow}^+(\omega)$ is obtained by calculating the matrix inverse $(\mathbf{M}^{-1})_{dd}$, where the subscript dd indicates the element obtained from $c_{d\uparrow}$ in both row and column. Calculating the inverse of an infinite-dimensional matrix \mathbf{M} is a nontrivial problem. For this purpose, we perform matrix reduction by using Löwdin's partitioning technique [21, 22]. We consider an eigenvalue equation $\mathbf{M}\mathbf{C} = \mathbf{0}$, in which the column vector $\mathbf{C} = (\mathbf{C}_L \mathbf{C}_d \mathbf{C}_R)^T$, where \mathbf{C}_L , \mathbf{C}_d , and \mathbf{C}_R correspond to the row vectors $(c_{k\uparrow}^L, \delta n_{d\downarrow} c_{k\uparrow}^L)$, $(\delta j_{d\downarrow}^{+L} c_{d\uparrow}, \delta j_{d\downarrow}^{-L} c_{d\uparrow}, c_{d\uparrow}, \delta j_{d\downarrow}^{-R} c_{d\uparrow}, \delta j_{d\downarrow}^{+R} c_{d\uparrow})$, and $(\delta n_{d\downarrow} c_{k\uparrow}^R, c_{k\uparrow}^R)$, respectively, and $\mathbf{0}$ is a column vector with zero elements. After eliminating \mathbf{C}_L and \mathbf{C}_R , we obtain an equation $(\mathbf{M}_d - \mathbf{M}_{Ld} \mathbf{M}_{LL}^{-1} \mathbf{M}_{dL} - \mathbf{M}_{Rd} \mathbf{M}_{RR}^{-1} \mathbf{M}_{dR}) \mathbf{C}_d \equiv \mathbf{M}_r \mathbf{C}_d = \mathbf{0}$, which leads to

$$\mathbf{M}_r = \mathbf{M}_d - \mathbf{M}_{Ld} \mathbf{M}_{LL}^{-1} \mathbf{M}_{dL} - \mathbf{M}_{Rd} \mathbf{M}_{RR}^{-1} \mathbf{M}_{dR}. \quad (20)$$

The last two terms in Eq. (20) contribute to the self-energy of the retarded Green's function. We finally obtain \mathbf{M}_r for the two-reservoir Anderson model as follows:

$$\mathbf{M}_r = \begin{pmatrix} -i\omega' & -\gamma_{LL} & U_{J-}^L & \gamma_{LR} & \gamma_{J-} \\ \gamma_{LL} & -i\omega' & U_{J+}^L & \gamma_{J+} & \gamma_{LR} \\ -U_{J-}^{L*} & -U_{J+}^{L*} & -i\omega' & -U_{J+}^{R*} & -U_{J-}^{R*} \\ -\gamma_{LR} & -\gamma_{J-} & U_{J+}^R & -i\omega' & \gamma_{RR} \\ -\gamma_{J+} & -\gamma_{LR} & U_{J-}^R & -\gamma_{RR} & -i\omega' \end{pmatrix}. \quad (21)$$

Here, $\omega' \equiv \omega - \epsilon_d - U \langle n_{d\downarrow} \rangle$, where ϵ_d , U , and $\langle n_{d\downarrow} \rangle$ denote the energy level of the Kondo impurity, Coulomb interaction, and the average number of down-spin electrons occupying the level ϵ_d , respectively. The derivations of matrix elements are given in Appendix A. All the matrix elements, except the eight U -elements, have additional self-energy terms $i\Sigma_{mn} = \beta_{mn}(i\Sigma_0^L(\omega) + i\Sigma_0^R(\omega)) = 2\beta_{mn}\Delta$, where $\Sigma_0^L(\omega) = \sum_{\mathbf{k}} |V_{kd}^L|^2 / (\omega - \epsilon_{\mathbf{k}} + i\eta) = -i\Delta^L$ for a flat wide-band and $\Delta \equiv (\Delta^L + \Delta^R)/2$. Δ is used as a unit of energy. The lead function $\Gamma^L(\omega)$ in Eq. (1) is equal to $2\Delta^L$ in this study. The coefficients β_{mn} are $\beta_{11} = |\xi_d^{-L}|^2$, $\beta_{22} = |\xi_d^{+L}|^2$, $\beta_{33} = 1$, $\beta_{44} = |\xi_d^{+R}|^2$, $\beta_{55} = |\xi_d^{-R}|^2$, $\beta_{12(21)} = [\xi_d^{-L*} \xi_d^{+L}]^{(*)}$, $\beta_{14(41)} = [\xi_d^{-L*} \xi_d^{+R}]^{(*)}$, $\beta_{15(51)} = [\xi_d^{-L*} \xi_d^{-R}]^{(*)}$, $\beta_{24(42)} = [\xi_d^{+L*} \xi_d^{+R}]^{(*)}$, $\beta_{25(52)} = [\xi_d^{+L*} \xi_d^{-R}]^{(*)}$, and $\beta_{45(54)} = [\xi_d^{+R*} \xi_d^{-R}]^{(*)}$, where $\xi_d^{\mp L}$, for example, is expressed as

$$\begin{aligned} \xi_d^{\mp L} &= \frac{1}{2} \frac{\langle i[n_{d\downarrow}, j_{d\downarrow}^{\mp L}](1 - 2n_{d\uparrow}) \rangle + i(1 - 2\langle n_{d\downarrow} \rangle) \langle j_{d\downarrow}^{\mp L} \rangle}{\langle (\delta j_{d\downarrow}^{\mp L})^2 \rangle^{1/2} \langle (\delta n_{d\downarrow})^2 \rangle^{1/2}} \\ &= U_{J\mp}^L / [U \langle (\delta n_{d\downarrow})^2 \rangle^{1/2}]. \end{aligned} \quad (22)$$

We show the explicit expressions of β_{mn} in Appendix B.

The matrix elements represented by γ are written as

$$\begin{aligned} \gamma_{LL(RR)} &= \langle \sum_k i(V_{kd}^* c_{k\uparrow}^L + V_{kd}^* c_{k\uparrow}^R) c_{d\uparrow}^\dagger [j_{d\downarrow}^{-L(R)}, j_{d\downarrow}^{+L(R)}] \rangle \\ &\times [(\langle (\delta j_{d\downarrow}^{-L(R)})^2 \rangle) \langle (\delta j_{d\downarrow}^{+L(R)})^2 \rangle]^{-1/2}, \end{aligned} \quad (23)$$

$$\begin{aligned} \gamma_{J\mp} &= \langle \sum_k i(V_{kd}^* c_{k\uparrow}^L + V_{kd}^* c_{k\uparrow}^R) c_{d\uparrow}^\dagger [j_{d\downarrow}^{\mp L}, j_{d\downarrow}^{\mp R}] \rangle \\ &\times [(\langle (\delta j_{d\downarrow}^{\mp L})^2 \rangle) \langle (\delta j_{d\downarrow}^{\mp R})^2 \rangle]^{-1/2}, \end{aligned} \quad (24)$$

and

$$\begin{aligned} \gamma_{LR} &= \langle \sum_k i(V_{kd}^* c_{k\uparrow}^L + V_{kd}^* c_{k\uparrow}^R) c_{d\uparrow}^\dagger [j_{d\downarrow}^{-L}, j_{d\downarrow}^{+R}] \rangle \\ &\times [(\langle (\delta j_{d\downarrow}^{-L})^2 \rangle) \langle (\delta j_{d\downarrow}^{+R})^2 \rangle]^{-1/2}. \end{aligned} \quad (25)$$

We show the detailed derivations in Appendix A. The retarded Green's function $iG_{dd\uparrow}^+(\omega) = (\mathbf{M}_r^{-1})_{33}$ may explain all the features of nonlinear conductance observed in a quantum point contact[1–4], a single electron transistor[5–8], and scanning tunneling microscopy on a magnetic atom adsorbed on a metallic substrate[9–12].

In Fig. 1, we present the graphical illustrations of γ on the basis of the corresponding operator expressions, which are third-order processes of hybridization. Figure 1 depicts the Kondo processes in which a down-spin indicated by ① first enters the Kondo impurity and forms a singlet with an up-spin electron indicated by ②. Then, it performs an exchange process or singlet hopping. Figure 1 (a) describes the spin movements in γ_{LL} (left) and γ_{RR} (right) in equilibrium, and Fig. 1 (b), those in γ_{LR} (+) and γ_J (−). Each γ is composed of two terms, i.e., spin exchange and singlet hopping. The latter is a unique property of a two-reservoir system. It is noteworthy that

FIG. 1: Motions of electrons indicated in γ . (a) Kondo processes described by γ_{LL} (left) and γ_{RR} (right). The solid dot indicates a Kondo impurity. The up- and down-spin motions denoted by $\textcircled{2}$ on the same side represent the exchange process while the up- and down-spin motions denoted by $\textcircled{2}$ on different sides indicate singlet hopping. (b) Kondo processes of connecting mechanism: γ_{LR} (+ sign) and γ_J (- sign). (c) Unidirectional resonant tunneling of a singlet establishing current flow.

γ_{LL} and γ_{RR} represent the degree of Kondo coupling, whereas γ_{LR} and γ_J represent the resonant tunneling between two reservoirs.

The effect of bias is contained in the Fermi distribution function and is observed in the calculation of the expectation values of γ . In the ground state, resonant tunneling from the reservoir at lower chemical potential to the one at higher chemical potential is prohibited. Therefore, the second part of Fig. 1 (b) vanishes. The motion that establishes current flow in both γ_{LR} and γ_J is unidirectional, as shown in Fig. 1 (c), which leads to the condition $\gamma_{LR} = \gamma_J$. However, when the second part of Fig. 1 (b) does not vanish for certain reason, the condition $\gamma_{LR} > \gamma_J$ is obtained. In both conditions of γ , even the state of very low bias is quite different from that of zero bias at which $\gamma_J = 0$.

IV. SELF-CONSISTENT METHOD

The values of γ and the fluctuations in the denominators of Eqs. (22)–(25) may not be determined by direct calculation. These values can be determined by employing the self-consistent method, which was used by Nagaoka[23] for studying the conventional Kondo problem. However, we do not try to determine these values in this study. Nevertheless, in the following study, we consider them as free parameters in order to explain the experimental observations for a quantum point contact[1–4] and scanning tunneling microscopy[9–12].

Finally, we suggest a self-consistent scheme that is particularly useful when the application of a magnetic field disturbs the particle-hole symmetry. Because the matrix elements $U_{J\mp}^{L,R}$ and coefficients β_{mn} contain undetermined quantities $\langle n_{d\sigma} \rangle$, $\langle j_{d\sigma}^{-L,R} \rangle$, and $\langle j_{d\sigma}^{+L,R} \rangle$, and these

quantities are also expressed by the retarded Green's function such as

$$\langle n_{d\sigma} \rangle = -\frac{1}{\pi} \int_{-\infty}^{\infty} \frac{f_L(\omega)\Gamma^L(\omega) + f_R(\omega)\Gamma^R(\omega)}{\Gamma^L(\omega) + \Gamma^R(\omega)} \times \text{Im } G_{dd\sigma}^+(\omega) d\omega; \quad (26)$$

$$\langle j_{d\sigma}^{-L} \rangle = -\frac{1}{\pi} \int \frac{d\omega}{2} [f_L(\omega) - f_R(\omega)] \tilde{\Gamma}(\omega) \times \text{Im } G_{dd\sigma}^+(\omega) = -\langle j_{d\sigma}^{-R} \rangle; \quad (27)$$

$$\langle j_{d\sigma}^{+L(R)} \rangle = \int_{-\infty}^{\infty} \frac{d\omega}{\pi} f_{L(R)}(\omega) \Gamma^{L(R)}(\omega) \text{Re } G_{dd\sigma}^+(\omega), \quad (28)$$

where $\tilde{\Gamma}(\omega) = \Gamma^L(\omega)\Gamma^R(\omega)/[\Gamma^L(\omega) + \Gamma^R(\omega)]$, one can construct a self-consistent loop to obtain the retarded Green's function as follows:

$$\begin{aligned} \langle n_{d\downarrow} \rangle^{(0)}, \langle j_{d\downarrow}^{\mp L,R} \rangle^{(0)} &\rightarrow G_{dd\uparrow}^{+(0)}(\omega) \rightarrow \rho_{\uparrow}^{(0)}(\omega) \rightarrow \\ \langle n_{d\uparrow} \rangle^{(0)}, \langle j_{d\uparrow}^{\mp L,R} \rangle^{(0)} &\rightarrow G_{dd\downarrow}^{+(0)}(\omega) \rightarrow \rho_{\downarrow}^{(0)}(\omega) \rightarrow \\ \langle n_{d\downarrow} \rangle^{(1)}, \langle j_{d\downarrow}^{\mp L,R} \rangle^{(1)} &\rightarrow G_{dd\uparrow}^{+(1)}(\omega) \rightarrow \rho_{\uparrow}^{(1)}(\omega) \rightarrow \dots \end{aligned}$$

The expressions in Eqs. (26) and (27) are valid only when $\Gamma^L(\omega) \propto \Gamma^R(\omega)$. We report the results for the magnetic-field-induced peak splitting of the differential conductance in a single-electron transistor with a quantum dot[5–8] in terms of this self-consistent scheme in a separate study.

V. CONCLUSIONS

In conclusion, we have presented a systematic methodology for determining basis vectors spanning the Liouville space, which is the most crucial step in calculating the retarded Green's function using the resolvent operator; further, we have suggested a procedure for calculating the retarded Green's function. The operator method presented in this study has several advantages: (i) A complete set of basis vectors can be determined systematically, and (ii) the physical meanings of the basis vectors represented by the operators are apparent, allowing the identification and removal of the unimportant basis vectors for a particular parameter regime and subsequent construction of a reduced Liouville space. The on-site retarded Green's function for the single-impurity Anderson model with two metallic reservoirs is expressed as an inverse of a 5×5 matrix. We discussed the characteristics of the matrix elements under the application of a bias. Finally, we suggest a self-consistent calculation method that is useful when the system under consideration does not show particle-hole symmetry. This operator formulation for the retarded Green's function may be appropriate for studying the dynamics of a many-body system under steady-state nonequilibrium. In a separate study, we obtain the spectral function and differential conductance for a specific system that has a Kondo impurity between two metallic reservoirs under bias.

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Appendix A: Calculation of matrix elements

Calculation of the matrix elements of Eq. (19) for the single-impurity Anderson model with one reservoir in which γ_{LR} and γ_J^\mp do not appear is shown below. One can obtain the expressions of γ_{LR} and γ_J^\mp via the same manner shown here. The block $\mathbf{M}_{LL(RR)}$ comprises two diagonal blocks whose elements are the same and given by $-i\omega + i\epsilon_1 + 0^+$, $-i\omega + i\epsilon_2 + 0^+$, and so on. Since the calculation is very simple, we skip it.

(1) Matrix elements of the block \mathbf{M}_{Ld} :

Nontrivial elements of \mathbf{M}_{Ld} are

$$\begin{aligned} & -\langle \{i\mathbf{L}(c_{k\uparrow}\delta n_{d\downarrow}), \delta j_{d\downarrow}^\mp c_{d\uparrow}^\dagger\} \rangle, \text{ i.e., } \langle \{i[H, c_{k\uparrow}\delta n_{d\downarrow}], j_{d\downarrow}^\mp c_{d\uparrow}^\dagger\} \rangle \\ & = \langle \{i[H, c_{k\uparrow}]\delta n_{d\downarrow} + c_{k\uparrow}i[H, \delta n_{d\downarrow}], \delta j_{d\downarrow}^\mp c_{d\uparrow}^\dagger\} \rangle \\ & = -i\epsilon_k \langle \{c_{k\uparrow}\delta n_{d\downarrow}, \delta j_{d\downarrow}^\mp c_{d\uparrow}^\dagger\} \rangle - iV_{kd} \langle \{c_{d\uparrow}\delta n_{d\downarrow}, \delta j_{d\downarrow}^\mp c_{d\uparrow}^\dagger\} \rangle + \\ & \langle \{c_{k\uparrow}\delta j_{d\downarrow}^\mp, \delta j_{d\downarrow}^\mp c_{d\uparrow}^\dagger\} \rangle. \text{ The first term} \end{aligned}$$

$(-i\epsilon_k) \langle \{c_{k\uparrow}\delta n_{d\downarrow}, \delta j_{d\downarrow}^\mp c_{d\uparrow}^\dagger\} \rangle = (-i\epsilon_k) \langle [n_{d\downarrow}, j_{d\downarrow}^\mp] c_{k\uparrow} c_{d\uparrow}^\dagger \rangle$ should vanish because the up-spin dynamics of this form is not allowed. The third term also vanishes because $\langle \{c_{k\uparrow}j_{d\downarrow}^\mp, \delta j_{d\downarrow}^\mp c_{d\uparrow}^\dagger\} \rangle = \langle j_{d\downarrow}^\mp \delta j_{d\downarrow}^\mp \{c_{k\uparrow}, c_{d\uparrow}^\dagger\} \rangle = 0$. The second term, however, must be calculated rigorously, since it is a hybridization term that is related to the Kondo process. The operator $\{c_{d\uparrow}\delta n_{d\downarrow}, \delta j_{d\downarrow}^\mp c_{d\uparrow}^\dagger\}$ is expanded as $c_{d\uparrow}[\delta n_{d\downarrow}, \delta j_{d\downarrow}^\mp c_{d\uparrow}^\dagger] + [\delta j_{d\downarrow}^\mp c_{d\uparrow}^\dagger, c_{d\uparrow}]\delta n_{d\downarrow} + 2c_{d\uparrow}\delta j_{d\downarrow}^\mp c_{d\uparrow}^\dagger\delta n_{d\downarrow}$. Each term is rewritten as $c_{d\uparrow}[\delta n_{d\downarrow}, \delta j_{d\downarrow}^\mp c_{d\uparrow}^\dagger] = c_{d\uparrow}[n_{d\downarrow}, j_{d\downarrow}^\mp]c_{d\uparrow}^\dagger = c_{d\uparrow}c_{d\uparrow}^\dagger[n_{d\downarrow}, j_{d\downarrow}^\mp] = (1-n_{d\uparrow})[n_{d\downarrow}, j_{d\downarrow}^\mp]$ and $[\delta j_{d\downarrow}^\mp c_{d\uparrow}^\dagger, c_{d\uparrow}]\delta n_{d\downarrow} = \delta j_{d\downarrow}^\mp [c_{d\uparrow}^\dagger, c_{d\uparrow}]\delta n_{d\downarrow} = \delta j_{d\downarrow}^\mp (1-2c_{d\uparrow}c_{d\uparrow}^\dagger)\delta n_{d\downarrow}$. The last expression $-2c_{d\uparrow}\delta j_{d\downarrow}^\mp c_{d\uparrow}^\dagger\delta n_{d\downarrow}$ cancels the third term above. Hence, $-\langle \{i\mathbf{L}(c_{k\uparrow}\delta n_{d\downarrow}), j_{d\downarrow}^\mp c_{d\uparrow}^\dagger\} \rangle = iV_{kd} \langle (1-n_{d\uparrow})[n_{d\downarrow}, \delta j_{d\downarrow}^\mp] + \delta j_{d\downarrow}^\mp \delta n_{d\downarrow} \rangle = iV_{kd} \langle (\frac{1}{2}-n_{d\uparrow})[n_{d\downarrow}, j_{d\downarrow}^\mp] + \frac{1}{2}[n_{d\downarrow}, j_{d\downarrow}^\mp] + \delta j_{d\downarrow}^\mp \delta n_{d\downarrow} \rangle = \frac{iV_{kd}}{2} \langle (1-2n_{d\uparrow})[n_{d\downarrow}, j_{d\downarrow}^\mp] + \{\delta n_{d\downarrow}, \delta j_{d\downarrow}^\mp\} \rangle = \frac{iV_{kd}}{2} \langle (1-2n_{d\uparrow})[n_{d\downarrow}, j_{d\downarrow}^\mp] + (1-2\langle n_{d\downarrow} \rangle)\langle j_{d\downarrow}^\mp \rangle \rangle$.

Therefore, the matrix elements

$$\begin{aligned} & -\langle \{i\mathbf{L}(c_{k\uparrow}\delta n_{d\downarrow}), \delta j_{d\downarrow}^\mp c_{d\uparrow}^\dagger\} \rangle / [\|c_{k\uparrow}\delta n_{d\downarrow}\| \times \|c_{d\uparrow}\delta j_{d\downarrow}^\mp\|] = \\ & V_{kd}\xi_d^\mp, \text{ where } \xi_d^\mp = \frac{1}{2} \langle \{i(1-2n_{d\uparrow})[n_{d\downarrow}, j_{d\downarrow}^\mp] + i(1-2\langle n_{d\downarrow} \rangle)\langle j_{d\downarrow}^\mp \rangle\} \rangle / \langle (\delta n_{d\downarrow})^2 \rangle^{-1/2} \langle (\delta j_{d\downarrow}^\mp)^2 \rangle^{-1/2}. \end{aligned}$$

(2) Matrix elements of the block \mathbf{M}_d :

(2-1) Diagonal elements:

By using the commutator expression $i[H, c_{d\uparrow}] = -i\sum_{\mathbf{k}} V_{\mathbf{k}d}^* c_{\mathbf{k}\uparrow} - i\epsilon_d c_{d\uparrow} - iU c_{d\uparrow} n_{d\downarrow}$, the diagonal elements of the block \mathbf{M}_d are given by

$$(A): -\langle \{i[H, c_{d\uparrow}], c_{d\uparrow}^\dagger\} \rangle = i\sum_{\mathbf{k}} V_{\mathbf{k}d}^* \langle \{c_{\mathbf{k}\uparrow}, c_{d\uparrow}^\dagger\} \rangle +$$

$$\begin{aligned} & i\epsilon_d \langle \{c_{d\uparrow}, c_{d\uparrow}^\dagger\} \rangle + iU \langle \{c_{d\uparrow} n_{d\downarrow}, c_{d\uparrow}^\dagger\} \rangle \\ & = i\epsilon_d + iU \langle \{c_{d\uparrow} n_{d\downarrow}, c_{d\uparrow}^\dagger\} \rangle = i\epsilon_d + iU \langle \{c_{d\uparrow}, c_{d\uparrow}^\dagger\} n_{d\downarrow} \rangle \\ & = i\epsilon_d + iU \langle n_{d\downarrow} \rangle, \text{ and} \\ (B): & -\langle \{i[H, c_{d\uparrow} \delta j_{d\downarrow}^\mp], (c_{d\uparrow} \delta j_{d\downarrow}^\mp)^\dagger\} \rangle \\ & = -\langle \{i[H, c_{d\uparrow}] \delta j_{d\downarrow}^\mp, \delta j_{d\downarrow}^\mp c_{d\uparrow}^\dagger\} \rangle - \langle \{c_{d\uparrow} i[H, \delta j_{d\downarrow}^\mp], \delta j_{d\downarrow}^\mp c_{d\uparrow}^\dagger\} \rangle. \\ \text{The first term of (B) is rewritten as} \\ & \langle \{i[H, c_{d\uparrow}] \delta j_{d\downarrow}^\mp, \delta j_{d\downarrow}^\mp c_{d\uparrow}^\dagger\} \rangle = \langle \{(-i\sum_{\mathbf{k}} V_{\mathbf{k}d}^* c_{\mathbf{k}\uparrow} - i\epsilon_d c_{d\uparrow} - \\ & iU c_{d\uparrow} n_{d\downarrow}) \delta j_{d\downarrow}^\mp, (c_{d\uparrow} \delta j_{d\downarrow}^\mp)^\dagger\} \rangle = -i\epsilon_d \langle \{c_{d\uparrow} \delta j_{d\downarrow}^\mp, \delta j_{d\downarrow}^\mp c_{d\uparrow}^\dagger\} \rangle - \\ & iU \langle \{c_{d\uparrow} n_{d\downarrow} \delta j_{d\downarrow}^\mp, \delta j_{d\downarrow}^\mp c_{d\uparrow}^\dagger\} \rangle. \text{ Applying the decoupling ap-} \\ \text{proximation, } n_{d\downarrow} \delta j_{d\downarrow}^\mp &= \langle n_{d\downarrow} \rangle \delta j_{d\downarrow}^\mp, \text{ to the } U\text{-term above} \\ \text{gives rise to a form of squared norm for the first term of} \\ (B), \text{ i.e., } \langle \{i[H, c_{d\uparrow}] \delta j_{d\downarrow}^\mp, \delta j_{d\downarrow}^\mp c_{d\uparrow}^\dagger\} \rangle &= [-i\epsilon_d - iU \langle n_{d\downarrow} \rangle] \times \\ & \|c_{d\uparrow} \delta j_{d\downarrow}^\mp\|^2. \text{ The second term of (B), however, cannot be} \\ \text{written in the form of a squared norm, because } [H, j_{d\downarrow}^\mp] &\propto j_{d\downarrow}^\pm. \text{ Therefore, we neglect it.} \end{aligned}$$

(2-2) Matrix elements $U_{J\mp}$:

These are given by the inner products

$$\begin{aligned} & -\langle \{i\mathbf{L}c_{d\uparrow}, \delta j_{d\downarrow}^\mp c_{d\uparrow}^\dagger\} \rangle, \text{ i.e., } -\langle \{i[H, c_{d\uparrow}], \delta j_{d\downarrow}^\mp c_{d\uparrow}^\dagger\} \rangle \\ & = i\epsilon_d \langle \delta j_{d\downarrow}^\mp \rangle \langle \{c_{d\uparrow}, c_{d\uparrow}^\dagger\} \rangle + iU \langle \{c_{d\uparrow} n_{d\downarrow}, \delta j_{d\downarrow}^\mp c_{d\uparrow}^\dagger\} \rangle \\ & + i\sum_{\mathbf{k}} V_{\mathbf{k}d}^* \langle \delta j_{d\downarrow}^\mp \rangle \langle \{c_{\mathbf{k}\uparrow}, c_{d\uparrow}^\dagger\} \rangle = iU \langle \{c_{d\uparrow} n_{d\downarrow}, \delta j_{d\downarrow}^\mp c_{d\uparrow}^\dagger\} \rangle. \\ \text{However, } \langle \{c_{d\uparrow} \delta n_{d\downarrow}, \delta j_{d\downarrow}^\mp c_{d\uparrow}^\dagger\} \rangle &= \langle c_{d\uparrow} [\delta n_{d\downarrow}, \delta j_{d\downarrow}^\mp c_{d\uparrow}^\dagger] \rangle + \\ & \langle [\delta j_{d\downarrow}^\mp c_{d\uparrow}^\dagger, c_{d\uparrow}] \delta n_{d\downarrow} \rangle + \langle 2c_{d\uparrow} \delta j_{d\downarrow}^\mp c_{d\uparrow}^\dagger \delta n_{d\downarrow} \rangle, \text{ where} \\ \text{the operator in the first term is rewritten as} \\ c_{d\uparrow} [\delta n_{d\downarrow}, \delta j_{d\downarrow}^\mp c_{d\uparrow}^\dagger] &= c_{d\uparrow} [n_{d\downarrow}, j_{d\downarrow}^\mp] c_{d\uparrow}^\dagger = c_{d\uparrow} c_{d\uparrow}^\dagger [n_{d\downarrow}, j_{d\downarrow}^\mp] = \\ (1-n_{d\uparrow})[n_{d\downarrow}, j_{d\downarrow}^\mp], \text{ while the second term is given} \\ \text{by } \langle [\delta j_{d\downarrow}^\mp c_{d\uparrow}^\dagger, c_{d\uparrow}] \delta n_{d\downarrow} \rangle &= \langle \delta j_{d\downarrow}^\mp [c_{d\uparrow}^\dagger, c_{d\uparrow}] \delta n_{d\downarrow} \rangle = \\ \langle \delta j_{d\downarrow}^\mp \delta n_{d\downarrow} \rangle - \langle 2\delta j_{d\downarrow}^\mp c_{d\uparrow} c_{d\uparrow}^\dagger \delta n_{d\downarrow} \rangle. \text{ The last one can-} \\ \text{cels the third term of } \langle \{c_{d\uparrow} \delta n_{d\downarrow}, \delta j_{d\downarrow}^\mp c_{d\uparrow}^\dagger\} \rangle &\text{ above. Hence,} \\ \langle \{c_{d\uparrow} \delta n_{d\downarrow}, \delta j_{d\downarrow}^\mp c_{d\uparrow}^\dagger\} \rangle &= \langle (1-n_{d\uparrow})[n_{d\downarrow}, j_{d\downarrow}^\mp] + \delta j_{d\downarrow}^\mp \delta n_{d\downarrow} \rangle = \\ \langle (\frac{1}{2}-n_{d\uparrow})[n_{d\downarrow}, j_{d\downarrow}^\mp] + \frac{1}{2}[\delta n_{d\downarrow}, \delta j_{d\downarrow}^\mp] + \delta j_{d\downarrow}^\mp \delta n_{d\downarrow} \rangle &= \\ \frac{1}{2} \langle (1-2n_{d\uparrow})[n_{d\downarrow}, j_{d\downarrow}^\mp] + \{\delta n_{d\downarrow}, \delta j_{d\downarrow}^\mp\} \rangle &= \frac{1}{2} \langle \{ (1-2n_{d\uparrow})[n_{d\downarrow}, j_{d\downarrow}^\mp] + (1-2\langle n_{d\downarrow} \rangle)\langle j_{d\downarrow}^\mp \rangle \} \rangle. \\ \text{Therefore, the matrix elements denoted by } U_{J\mp} &\text{ is given by} \end{aligned}$$

$$\begin{aligned} U_{J\mp} &= -\langle \{i\mathbf{L}c_{d\uparrow}, \delta j_{d\downarrow}^\mp c_{d\uparrow}^\dagger\} \rangle \langle (\delta j_{d\downarrow}^\mp)^2 \rangle^{-1/2} \\ &= \frac{iU}{2} \langle \{ (1-2n_{d\uparrow})[n_{d\downarrow}, j_{d\downarrow}^\mp] + (1-2\langle n_{d\downarrow} \rangle)\langle j_{d\downarrow}^\mp \rangle \} \rangle \langle (\delta j_{d\downarrow}^\mp)^2 \rangle^{-1/2}. \end{aligned}$$

(2-3) Matrix elements $\gamma_{LL(RR)}$:

The inner products $-\langle \{i\mathbf{L}(c_{d\uparrow} \delta j_{d\downarrow}^\mp), \delta j_{d\downarrow}^\pm c_{d\uparrow}^\dagger\} \rangle$ gives rise to the expressions for $\gamma_{LL(RR)}$. Since $\langle \{i\mathbf{L}(c_{d\uparrow} \delta j_{d\downarrow}^\mp), \delta j_{d\downarrow}^\pm c_{d\uparrow}^\dagger\} \rangle = \langle \{i[H, c_{d\uparrow}] \delta j_{d\downarrow}^\mp, \delta j_{d\downarrow}^\pm c_{d\uparrow}^\dagger\} \rangle + \langle \{c_{d\uparrow} i[H, \delta j_{d\downarrow}^\mp], \delta j_{d\downarrow}^\pm c_{d\uparrow}^\dagger\} \rangle$, the first term can be expanded as $\langle \{i[H, c_{d\uparrow}] \delta j_{d\downarrow}^\mp, \delta j_{d\downarrow}^\pm c_{d\uparrow}^\dagger\} \rangle = -i\epsilon_d \langle \{c_{d\uparrow} \delta j_{d\downarrow}^\mp, \delta j_{d\downarrow}^\pm c_{d\uparrow}^\dagger\} \rangle - iU \langle \{c_{d\uparrow} n_{d\downarrow} \delta j_{d\downarrow}^\mp, \delta j_{d\downarrow}^\pm c_{d\uparrow}^\dagger\} \rangle - i\sum_{\mathbf{k}} V_{\mathbf{k}d}^* \langle \{c_{\mathbf{k}\uparrow} \delta j_{d\downarrow}^\mp, \delta j_{d\downarrow}^\pm c_{d\uparrow}^\dagger\} \rangle$. The first and second terms of this expression should vanish because they are not written in the form of a squared norm. Since the third term describes the Kondo process, we treat it rigorously and have the following expression:

$-i \sum_{\mathbf{k}} V_{\mathbf{k}d}^* \langle \{c_{k\uparrow} \delta j_{d\downarrow}^{\mp}, \delta j_{d\downarrow}^{\pm} c_{d\uparrow}^{\dagger}\} \rangle$
 $= -i \sum_{\mathbf{k}} V_{\mathbf{k}d}^* \langle \{ \delta j_{d\downarrow}^{\mp} \delta j_{d\downarrow}^{\pm} c_{k\uparrow} c_{d\uparrow}^{\dagger} - \delta j_{d\downarrow}^{\pm} \delta j_{d\downarrow}^{\mp} c_{k\uparrow} c_{d\uparrow}^{\dagger} \} \rangle$
 $= -i \sum_{\mathbf{k}} V_{\mathbf{k}d}^* \langle [\delta j_{d\downarrow}^{\mp}, \delta j_{d\downarrow}^{\pm}] c_{k\uparrow} c_{d\uparrow}^{\dagger} \rangle$
 $= -i \sum_{\mathbf{k}} V_{\mathbf{k}d}^* \langle [j_{d\downarrow}^{\mp}, j_{d\downarrow}^{\pm}] c_{k\uparrow} c_{d\uparrow}^{\dagger} \rangle$. The second term of $\langle \{i\mathbf{L}(c_{d\uparrow} \delta j_{d\downarrow}^{\mp}, \delta j_{d\downarrow}^{\pm} c_{d\uparrow}^{\dagger})\} \rangle$, i.e., $\langle \{c_{d\uparrow} i[H, j_{d\downarrow}^{\mp}], \delta j_{d\downarrow}^{\pm} c_{d\uparrow}^{\dagger}\} \rangle$, is rather complicate because it contains the commutator $i[H, j_{d\downarrow}^{\mp}]$. This commutator is expanded as $i[H, j_{d\downarrow}^{\mp}] = \pm \epsilon_d j_{d\downarrow}^{\pm} \mp (i) \sum_k \epsilon_k (V_{kd} c_{k\downarrow}^{\dagger} c_{d\downarrow} \pm V_{kd}^* c_{d\downarrow}^{\dagger} c_{k\downarrow}) \pm U n_{d\uparrow} j_{d\downarrow}^{\pm} \pm (i) \sum_{k,\ell} (V_{kd} V_{\ell d} c_{k\downarrow}^{\dagger} c_{\ell\downarrow} \pm V_{kd}^* V_{\ell d}^* c_{\ell\downarrow}^{\dagger} c_{k\downarrow})$, where (i) is applied only to the lower signs and the prime in sum denotes $k \neq \ell$. The first two terms on the right side are cancelled if we assume $\epsilon_k \approx \epsilon_d$, and the U -term is neglected in the Kondo regime. The last term, second order hybridization, describes the round trip of a down-spin electron between the Kondo impurity and the lead, which is equivalent to $(j_{d\downarrow}^{\pm})^2$. Since we consider only single trip of a down-spin electron in this study, we neglect the term involving $[H, j_{d\downarrow}^{\mp}]$. Thus, the matrix element $(\mathbf{M}_d)_{21/12} = \frac{-\langle \{i\mathbf{L}(c_{d\uparrow} \delta j_{d\downarrow}^{\mp}, \delta j_{d\downarrow}^{\pm} c_{d\uparrow}^{\dagger})\} \rangle}{\sqrt{\langle (\delta j_{d\downarrow}^{\mp})^2 \rangle} \sqrt{\langle (\delta j_{d\downarrow}^{\pm})^2 \rangle}} = \pm \gamma$, where $\gamma = \pm \frac{i \sum_{\mathbf{k}} V_{\mathbf{k}d}^* \langle c_{k\uparrow} c_{d\uparrow}^{\dagger} [j_{d\downarrow}^{\mp}, j_{d\downarrow}^{\pm}] \rangle}{\sqrt{\langle (\delta j_{d\downarrow}^{\mp})^2 \rangle} \sqrt{\langle (\delta j_{d\downarrow}^{\pm})^2 \rangle}}$ for the single-reservoir Anderson model. $\gamma_{LL(RR)}$ for the two-reservoir Anderson model is given by

$$\gamma_{LL(RR)} = \frac{i \sum_{\mathbf{k}} V_{\mathbf{k}d}^* \langle c_{k\uparrow}^L c_{d\uparrow}^{\dagger} + c_{k\uparrow}^R c_{d\uparrow}^{\dagger} \rangle [j_{d\downarrow}^{-L(R)}, j_{d\downarrow}^{+L(R)}]}{\langle (\delta j_{d\downarrow}^{-L(R)})^2 \rangle^{1/2} \langle (\delta j_{d\downarrow}^{+L(R)})^2 \rangle^{1/2}}.$$

Appendix B: Expressions of β_{mn}

We obtain the expressions of β_{mn} in terms of the definitions and the expressions of ξ_i^{\mp} given in Eq. (22). The coefficients β_{mn} in front of the self-energy function, i.e., $i\Sigma_{mn}(\omega) = \beta_{mn}(i\Sigma_0^L(\omega) + i\Sigma_0^R(\omega))$, are symmetric in exchanging their indices. By using the operator identity $[n_{i\downarrow}, j_{i\downarrow}^{\mp}] = \mp i j_{i\downarrow}^{\pm}$, we write a different expression for $\text{Re}[U_{j\pm}^{\pm L, R}]$, i.e., $\text{Re}[U_{j\pm}^{\pm L, R}] \equiv (U/2\tau)$, where

$$1/\tau = [\pm \langle j_{i\downarrow}^{\pm L, R} \rangle \mp 2 \langle j_{i\downarrow}^{\pm L, R} n_{i\uparrow} \rangle] / \sqrt{\langle (\delta j_{i\downarrow}^{\mp L, R})^2 \rangle},$$

which will be used in the expressions of $\text{Re}[\beta_{mn}]$. The final forms of $\text{Re}[\beta_{mn}]$ are given by using $\langle (\delta n_{i\downarrow})^2 \rangle \approx 1/4$ and $\tau = 2$ that is the value at the atomic limit. Since $\langle j_{i\downarrow}^{+L(R)} \rangle < 0$ and $\langle j_{i\downarrow}^{-L} \rangle = -\langle j_{i\downarrow}^{-R} \rangle$, an inequality, $\text{Re}[\beta_{12(14)}] < \text{Re}[\beta_{15}] < \text{Re}[\beta_{11(55)}] < \text{Re}[\beta_{25(45)}] < \text{Re}[\beta_{22(44)}]$, exists. We obtain the expressions of β_{mn} as follows:

Real parts of β_{mn} :

$$\begin{aligned}
 \text{Re}[\beta_{11}] &= \text{Re}[\xi_L^{-*} \xi_L^+] = \\
 &= \left[\langle (j_{i\downarrow}^{+L} - 2\langle n_{i\uparrow} j_{i\downarrow}^{+L} \rangle)^2 + (1 - 2\langle n_{i\downarrow} \rangle)^2 \langle j_{i\downarrow}^{-L} \rangle^2 \right] \frac{[4\langle (\delta n_{i\downarrow})^2 \rangle]^{-1}}{\langle (\delta j_{i\downarrow}^{-L})^2 \rangle} \\
 &= \left[\frac{1}{\tau^2} + \frac{(1-2\langle n_{i\downarrow} \rangle)^2 \langle j_{i\downarrow}^{-L} \rangle^2}{\langle (\delta j_{i\downarrow}^{-L})^2 \rangle} \right] \frac{1}{4\langle (\delta n_{i\downarrow})^2 \rangle}
 \end{aligned}$$

$$\approx \left[\frac{1}{4} + \frac{(1-2\langle n_{i\downarrow} \rangle)^2 \langle j_{i\downarrow}^{-L} \rangle^2}{\langle (\delta j_{i\downarrow}^{-L})^2 \rangle} \right].$$

Only the index L changes to R for $\text{Re}[\beta_{55}]$.

$$\begin{aligned}
 \text{Re}[\beta_{22}] &= \text{Re}[\xi_L^{+*} \xi_L^+] = \\
 &= \left[\langle (j_{i\downarrow}^{-L} - 2\langle n_{i\uparrow} j_{i\downarrow}^{-L} \rangle)^2 + (1 - 2\langle n_{i\downarrow} \rangle)^2 \langle j_{i\downarrow}^{+L} \rangle^2 \right] \frac{[4\langle (\delta n_{i\downarrow})^2 \rangle]^{-1}}{\langle (\delta j_{i\downarrow}^{+L})^2 \rangle} \\
 &= \left[\frac{1}{\tau^2} + \frac{(1-2\langle n_{i\downarrow} \rangle)^2 \langle j_{i\downarrow}^{+L} \rangle^2}{\langle (\delta j_{i\downarrow}^{+L})^2 \rangle} \right] \frac{1}{4\langle (\delta n_{i\downarrow})^2 \rangle} \\
 &\approx \left[\frac{1}{4} + \frac{(1-2\langle n_{i\downarrow} \rangle)^2 \langle j_{i\downarrow}^{+L} \rangle^2}{\langle (\delta j_{i\downarrow}^{+L})^2 \rangle} \right].
 \end{aligned}$$

Here, again, the index L changes to R for $\text{Re}[\beta_{44}]$.

$$\begin{aligned}
 \text{Re}[\beta_{12}] &= \text{Re}[\xi_L^{-*} \xi_L^+] = \text{Re}[\beta_{21}] = \\
 &= \left[\langle (j_{i\downarrow}^{+L} - 2\langle n_{i\uparrow} j_{i\downarrow}^{+L} \rangle)(- \langle j_{i\downarrow}^{-L} \rangle + 2\langle n_{i\uparrow} j_{i\downarrow}^{-L} \rangle) \right. \\
 &\quad \left. + (1 - 2\langle n_{i\downarrow} \rangle)^2 \langle j_{i\downarrow}^{-L} \rangle \langle j_{i\downarrow}^{+L} \rangle \right] \frac{[4\langle (\delta n_{i\downarrow})^2 \rangle]^{-1}}{\sqrt{\langle (\delta j_{i\downarrow}^{-L})^2 \rangle} \sqrt{\langle (\delta j_{i\downarrow}^{+L})^2 \rangle}} \\
 &= \left[\frac{1}{\tau^2} + \frac{(1-2\langle n_{i\downarrow} \rangle)^2 \langle j_{i\downarrow}^{-L} \rangle \langle j_{i\downarrow}^{+L} \rangle}{\sqrt{\langle (\delta j_{i\downarrow}^{-L})^2 \rangle} \sqrt{\langle (\delta j_{i\downarrow}^{+L})^2 \rangle}} \right] \frac{1}{4\langle (\delta n_{i\downarrow})^2 \rangle} \\
 &\approx \left[\frac{1}{4} + \frac{(1-2\langle n_{i\downarrow} \rangle)^2 \langle j_{i\downarrow}^{-L} \rangle \langle j_{i\downarrow}^{+L} \rangle}{\sqrt{\langle (\delta j_{i\downarrow}^{-L})^2 \rangle} \sqrt{\langle (\delta j_{i\downarrow}^{+L})^2 \rangle}} \right],
 \end{aligned}$$

$$\begin{aligned}
 \text{Re}[\beta_{14}] &= \text{Re}[\xi_L^{-*} \xi_R^+] = \text{Re}[\beta_{41}] = \\
 &= \left[\langle (j_{i\downarrow}^{+L} - 2\langle n_{i\uparrow} j_{i\downarrow}^{+L} \rangle)(- \langle j_{i\downarrow}^{-R} \rangle + 2\langle n_{i\uparrow} j_{i\downarrow}^{-R} \rangle) \right. \\
 &\quad \left. + (1 - 2\langle n_{i\downarrow} \rangle)^2 \langle j_{i\downarrow}^{-L} \rangle \langle j_{i\downarrow}^{+R} \rangle \right] \frac{[4\langle (\delta n_{i\downarrow})^2 \rangle]^{-1}}{\sqrt{\langle (\delta j_{i\downarrow}^{-L})^2 \rangle} \sqrt{\langle (\delta j_{i\downarrow}^{+R})^2 \rangle}} \\
 &= \left[\frac{1}{\tau^2} + \frac{(1-2\langle n_{i\downarrow} \rangle)^2 \langle j_{i\downarrow}^{-L} \rangle \langle j_{i\downarrow}^{+R} \rangle}{\sqrt{\langle (\delta j_{i\downarrow}^{-L})^2 \rangle} \sqrt{\langle (\delta j_{i\downarrow}^{+R})^2 \rangle}} \right] \frac{1}{4\langle (\delta n_{i\downarrow})^2 \rangle} \\
 &\approx \left[\frac{1}{4} + \frac{(1-2\langle n_{i\downarrow} \rangle)^2 \langle j_{i\downarrow}^{-L} \rangle \langle j_{i\downarrow}^{+R} \rangle}{\sqrt{\langle (\delta j_{i\downarrow}^{-L})^2 \rangle} \sqrt{\langle (\delta j_{i\downarrow}^{+R})^2 \rangle}} \right],
 \end{aligned}$$

$$\begin{aligned}
 \text{Re}[\beta_{15}] &= \text{Re}[\xi_L^{-*} \xi_R^-] = \text{Re}[\beta_{51}] = \\
 &= \left[\langle (j_{i\downarrow}^{+L} - 2\langle n_{i\uparrow} j_{i\downarrow}^{+L} \rangle)(\langle j_{i\downarrow}^{+R} \rangle - 2\langle n_{i\uparrow} j_{i\downarrow}^{+R} \rangle) \right. \\
 &\quad \left. + (1 - 2\langle n_{i\downarrow} \rangle)^2 \langle j_{i\downarrow}^{-L} \rangle \langle j_{i\downarrow}^{-R} \rangle \right] \frac{[4\langle (\delta n_{i\downarrow})^2 \rangle]^{-1}}{\sqrt{\langle (\delta j_{i\downarrow}^{-L})^2 \rangle} \sqrt{\langle (\delta j_{i\downarrow}^{-R})^2 \rangle}} \\
 &= \left[\frac{1}{\tau^2} + \frac{(1-2\langle n_{i\downarrow} \rangle)^2 \langle j_{i\downarrow}^{-L} \rangle \langle j_{i\downarrow}^{-R} \rangle}{\sqrt{\langle (\delta j_{i\downarrow}^{-L})^2 \rangle} \sqrt{\langle (\delta j_{i\downarrow}^{-R})^2 \rangle}} \right] \frac{1}{4\langle (\delta n_{i\downarrow})^2 \rangle} \\
 &\approx \left[\frac{1}{4} + \frac{(1-2\langle n_{i\downarrow} \rangle)^2 \langle j_{i\downarrow}^{-L} \rangle \langle j_{i\downarrow}^{-R} \rangle}{\sqrt{\langle (\delta j_{i\downarrow}^{-L})^2 \rangle} \sqrt{\langle (\delta j_{i\downarrow}^{-R})^2 \rangle}} \right],
 \end{aligned}$$

$$\begin{aligned}
 \text{Re}[\beta_{24}] &= \text{Re}[\xi_L^{+*} \xi_R^+] = \text{Re}[\beta_{42}] = \\
 &= \left[\langle (2\langle n_{i\uparrow} j_{i\downarrow}^{-L} \rangle - \langle j_{i\downarrow}^{-L} \rangle)(2\langle n_{i\uparrow} j_{i\downarrow}^{-R} \rangle - \langle j_{i\downarrow}^{-R} \rangle) \right. \\
 &\quad \left. + (1 - 2\langle n_{i\downarrow} \rangle)^2 \langle j_{i\downarrow}^{+L} \rangle \langle j_{i\downarrow}^{+R} \rangle \right] \frac{[4\langle (\delta n_{i\downarrow})^2 \rangle]^{-1}}{\sqrt{\langle (\delta j_{i\downarrow}^{+L})^2 \rangle} \sqrt{\langle (\delta j_{i\downarrow}^{+R})^2 \rangle}} \\
 &= \left[\frac{1}{\tau^2} + \frac{(1-2\langle n_{i\downarrow} \rangle)^2 \langle j_{i\downarrow}^{+L} \rangle \langle j_{i\downarrow}^{+R} \rangle}{\sqrt{\langle (\delta j_{i\downarrow}^{+L})^2 \rangle} \sqrt{\langle (\delta j_{i\downarrow}^{+R})^2 \rangle}} \right] \frac{1}{4\langle (\delta n_{i\downarrow})^2 \rangle} \\
 &\approx \left[\frac{1}{4} + \frac{(1-2\langle n_{i\downarrow} \rangle)^2 \langle j_{i\downarrow}^{+L} \rangle \langle j_{i\downarrow}^{+R} \rangle}{\sqrt{\langle (\delta j_{i\downarrow}^{+L})^2 \rangle} \sqrt{\langle (\delta j_{i\downarrow}^{+R})^2 \rangle}} \right],
 \end{aligned}$$

$$\begin{aligned}
 \text{Re}[\beta_{25}] &= \text{Re}[\xi_L^{+*} \xi_R^-] = \text{Re}[\beta_{52}] = \\
 &= \left[\langle (- \langle j_{i\downarrow}^{-L} \rangle + 2\langle n_{i\uparrow} j_{i\downarrow}^{-L} \rangle)(\langle j_{i\downarrow}^{+R} \rangle - 2\langle n_{i\uparrow} j_{i\downarrow}^{+R} \rangle) \right.
 \end{aligned}$$

$$\begin{aligned}
& + (1 - 2\langle n_{i\downarrow} \rangle)^2 \langle j_{i\downarrow}^{+L} \rangle \langle j_{i\downarrow}^{-R} \rangle \left] \frac{[4\langle (\delta n_{i\downarrow})^2 \rangle]^{-1}}{\sqrt{\langle (\delta j_{i\downarrow}^{+L})^2 \rangle} \sqrt{\langle (\delta j_{i\downarrow}^{-R})^2 \rangle}} \right. \\
& = \left[\frac{1}{\tau^2} + \frac{(1-2\langle n_{i\downarrow} \rangle)^2 \langle j_{i\downarrow}^{+L} \rangle \langle j_{i\downarrow}^{-R} \rangle}{\sqrt{\langle (\delta j_{i\downarrow}^{+L})^2 \rangle} \sqrt{\langle (\delta j_{i\downarrow}^{-R})^2 \rangle}} \right] \frac{1}{4\langle (\delta n_{i\downarrow})^2 \rangle} \\
& \approx \left[\frac{1}{4} + \frac{(1-2\langle n_{i\downarrow} \rangle)^2 \langle j_{i\downarrow}^{+L} \rangle \langle j_{i\downarrow}^{-R} \rangle}{\sqrt{\langle (\delta j_{i\downarrow}^{+L})^2 \rangle} \sqrt{\langle (\delta j_{i\downarrow}^{-R})^2 \rangle}} \right],
\end{aligned}$$

$$\begin{aligned}
\text{Re}[\beta_{45}] &= \text{Re}[\xi_R^{+*} \xi_R^-] = \text{Re}[\beta_{54}] = \\
& \left[(-\langle j_{i\downarrow}^{-R} \rangle + 2\langle n_{i\uparrow} j_{i\downarrow}^{-R} \rangle) (\langle j_{i\downarrow}^{+R} \rangle - 2\langle n_{i\uparrow} j_{i\downarrow}^{+R} \rangle) \right. \\
& + (1 - 2\langle n_{i\downarrow} \rangle)^2 \langle j_{i\downarrow}^{+R} \rangle \langle j_{i\downarrow}^{-R} \rangle \left. \right] \frac{[4\langle (\delta n_{i\downarrow})^2 \rangle]^{-1}}{\sqrt{\langle (\delta j_{i\downarrow}^{+R})^2 \rangle} \sqrt{\langle (\delta j_{i\downarrow}^{-R})^2 \rangle}} \\
& = \left[\frac{1}{\tau^2} + \frac{(1-2\langle n_{i\downarrow} \rangle)^2 \langle j_{i\downarrow}^{+R} \rangle \langle j_{i\downarrow}^{-R} \rangle}{\sqrt{\langle (\delta j_{i\downarrow}^{+R})^2 \rangle} \sqrt{\langle (\delta j_{i\downarrow}^{-R})^2 \rangle}} \right] \frac{1}{4\langle (\delta n_{i\downarrow})^2 \rangle} \\
& \approx \left[\frac{1}{4} + \frac{(1-2\langle n_{i\downarrow} \rangle)^2 \langle j_{i\downarrow}^{+R} \rangle \langle j_{i\downarrow}^{-R} \rangle}{\sqrt{\langle (\delta j_{i\downarrow}^{+R})^2 \rangle} \sqrt{\langle (\delta j_{i\downarrow}^{-R})^2 \rangle}} \right].
\end{aligned}$$

Imaginary parts of β_{mn} :

$$\begin{aligned}
\text{Im}[\beta_{12}] &= \text{Im}[\xi_L^{+*} \xi_L^+] \\
&= \frac{(1-2\langle n_{i\downarrow} \rangle)}{4\langle (\delta n_{i\downarrow})^2 \rangle} \left[\frac{\langle j_{i\downarrow}^{+L} \rangle - 2\langle n_{i\uparrow} j_{i\downarrow}^{+L} \rangle}{\sqrt{\langle (\delta j_{i\downarrow}^{+L})^2 \rangle}} \frac{\langle j_{i\downarrow}^{+L} \rangle}{\sqrt{\langle (\delta j_{i\downarrow}^{+L})^2 \rangle}} \right. \\
& \quad \left. - \frac{-\langle j_{i\downarrow}^{-L} \rangle + 2\langle n_{i\uparrow} j_{i\downarrow}^{-L} \rangle}{\sqrt{\langle (\delta j_{i\downarrow}^{+L})^2 \rangle}} \frac{\langle j_{i\downarrow}^{-L} \rangle}{\sqrt{\langle (\delta j_{i\downarrow}^{+L})^2 \rangle}} \right] \\
&= \frac{(1-2\langle n_{i\downarrow} \rangle)}{4\langle (\delta n_{i\downarrow})^2 \rangle} \frac{1}{\tau} \left[\frac{\langle j_{i\downarrow}^{+L} \rangle}{\sqrt{\langle (\delta j_{i\downarrow}^{+L})^2 \rangle}} - \frac{\langle j_{i\downarrow}^{-L} \rangle}{\sqrt{\langle (\delta j_{i\downarrow}^{+L})^2 \rangle}} \right]
\end{aligned}$$

$$\begin{aligned}
\text{Im}[\beta_{14}] &= \text{Im}[\xi_L^{+*} \xi_R^+] \\
&= \frac{(1-2\langle n_{i\downarrow} \rangle)}{4\langle (\delta n_{i\downarrow})^2 \rangle} \left[\frac{\langle j_{i\downarrow}^{+L} \rangle - 2\langle n_{i\uparrow} j_{i\downarrow}^{+L} \rangle}{\sqrt{\langle (\delta j_{i\downarrow}^{+L})^2 \rangle}} \frac{\langle j_{i\downarrow}^{+R} \rangle}{\sqrt{\langle (\delta j_{i\downarrow}^{+R})^2 \rangle}} \right. \\
& \quad \left. - \frac{-\langle j_{i\downarrow}^{-R} \rangle + 2\langle n_{i\uparrow} j_{i\downarrow}^{-R} \rangle}{\sqrt{\langle (\delta j_{i\downarrow}^{+R})^2 \rangle}} \frac{\langle j_{i\downarrow}^{-L} \rangle}{\sqrt{\langle (\delta j_{i\downarrow}^{+R})^2 \rangle}} \right] \\
&= \frac{(1-2\langle n_{i\downarrow} \rangle)}{4\langle (\delta n_{i\downarrow})^2 \rangle} \frac{1}{\tau} \left[\frac{\langle j_{i\downarrow}^{+R} \rangle}{\sqrt{\langle (\delta j_{i\downarrow}^{+R})^2 \rangle}} - \frac{\langle j_{i\downarrow}^{-L} \rangle}{\sqrt{\langle (\delta j_{i\downarrow}^{+R})^2 \rangle}} \right]
\end{aligned}$$

$$\begin{aligned}
\text{Im}[\beta_{15}] &= \text{Im}[\xi_L^{+*} \xi_R^-] \\
&= \frac{(1-2\langle n_{i\downarrow} \rangle)}{4\langle (\delta n_{i\downarrow})^2 \rangle} \left[\frac{\langle j_{i\downarrow}^{+L} \rangle - 2\langle n_{i\uparrow} j_{i\downarrow}^{+L} \rangle}{\sqrt{\langle (\delta j_{i\downarrow}^{+L})^2 \rangle}} \frac{\langle j_{i\downarrow}^{-R} \rangle}{\sqrt{\langle (\delta j_{i\downarrow}^{-R})^2 \rangle}} \right. \\
& \quad \left. - \frac{\langle j_{i\downarrow}^{+R} \rangle - 2\langle n_{i\uparrow} j_{i\downarrow}^{+R} \rangle}{\sqrt{\langle (\delta j_{i\downarrow}^{-R})^2 \rangle}} \frac{\langle j_{i\downarrow}^{-L} \rangle}{\sqrt{\langle (\delta j_{i\downarrow}^{-L})^2 \rangle}} \right] \\
&= \frac{(1-2\langle n_{i\downarrow} \rangle)}{4\langle (\delta n_{i\downarrow})^2 \rangle} \frac{1}{\tau} \left[\frac{\langle j_{i\downarrow}^{-R} \rangle}{\sqrt{\langle (\delta j_{i\downarrow}^{-R})^2 \rangle}} - \frac{\langle j_{i\downarrow}^{-L} \rangle}{\sqrt{\langle (\delta j_{i\downarrow}^{-L})^2 \rangle}} \right],
\end{aligned}$$

$$\begin{aligned}
\text{Im}[\beta_{25}] &= \frac{(1-2\langle n_{i\downarrow} \rangle)}{4\langle (\delta n_{i\downarrow})^2 \rangle} \left[\frac{-\langle j_{i\downarrow}^{-L} \rangle + 2\langle n_{i\uparrow} j_{i\downarrow}^{-L} \rangle}{\sqrt{\langle (\delta j_{i\downarrow}^{+L})^2 \rangle}} \frac{\langle j_{i\downarrow}^{-R} \rangle}{\sqrt{\langle (\delta j_{i\downarrow}^{-R})^2 \rangle}} \right. \\
& \quad \left. - \frac{\langle j_{i\downarrow}^{+R} \rangle - 2\langle n_{i\uparrow} j_{i\downarrow}^{+R} \rangle}{\sqrt{\langle (\delta j_{i\downarrow}^{-R})^2 \rangle}} \frac{\langle j_{i\downarrow}^{+L} \rangle}{\sqrt{\langle (\delta j_{i\downarrow}^{+L})^2 \rangle}} \right] \\
&= \frac{(1-2\langle n_{i\downarrow} \rangle)}{4\langle (\delta n_{i\downarrow})^2 \rangle} \frac{1}{\tau} \left[\frac{\langle j_{i\downarrow}^{-R} \rangle}{\sqrt{\langle (\delta j_{i\downarrow}^{-R})^2 \rangle}} - \frac{\langle j_{i\downarrow}^{+L} \rangle}{\sqrt{\langle (\delta j_{i\downarrow}^{+L})^2 \rangle}} \right],
\end{aligned}$$

$$\begin{aligned}
\text{Im}[\beta_{45}] &= \frac{(1-2\langle n_{i\downarrow} \rangle)}{4\langle (\delta n_{i\downarrow})^2 \rangle} \left[\frac{-\langle j_{i\downarrow}^{-R} \rangle + 2\langle n_{i\uparrow} j_{i\downarrow}^{-R} \rangle}{\sqrt{\langle (\delta j_{i\downarrow}^{+R})^2 \rangle}} \frac{\langle j_{i\downarrow}^{-R} \rangle}{\sqrt{\langle (\delta j_{i\downarrow}^{-R})^2 \rangle}} \right. \\
& \quad \left. - \frac{\langle j_{i\downarrow}^{+R} \rangle - 2\langle n_{i\uparrow} j_{i\downarrow}^{+R} \rangle}{\sqrt{\langle (\delta j_{i\downarrow}^{-R})^2 \rangle}} \frac{\langle j_{i\downarrow}^{+R} \rangle}{\sqrt{\langle (\delta j_{i\downarrow}^{+R})^2 \rangle}} \right] \\
&= \frac{(1-2\langle n_{i\downarrow} \rangle)}{4\langle (\delta n_{i\downarrow})^2 \rangle} \frac{1}{\tau} \left[\frac{\langle j_{i\downarrow}^{-R} \rangle}{\sqrt{\langle (\delta j_{i\downarrow}^{-R})^2 \rangle}} - \frac{\langle j_{i\downarrow}^{+R} \rangle}{\sqrt{\langle (\delta j_{i\downarrow}^{+R})^2 \rangle}} \right], \text{ and}
\end{aligned}$$

$$\begin{aligned}
\text{Im}[\beta_{24}] &= \frac{(1-2\langle n_{i\downarrow} \rangle)}{4\langle (\delta n_{i\downarrow})^2 \rangle} \left[\frac{-\langle j_{i\downarrow}^{-L} \rangle + 2\langle n_{i\uparrow} j_{i\downarrow}^{-L} \rangle}{\sqrt{\langle (\delta j_{i\downarrow}^{+L})^2 \rangle}} \frac{\langle j_{i\downarrow}^{+R} \rangle}{\sqrt{\langle (\delta j_{i\downarrow}^{+R})^2 \rangle}} \right. \\
& \quad \left. - \frac{-\langle j_{i\downarrow}^{-R} \rangle + 2\langle n_{i\uparrow} j_{i\downarrow}^{-R} \rangle}{\sqrt{\langle (\delta j_{i\downarrow}^{+R})^2 \rangle}} \frac{\langle j_{i\downarrow}^{+L} \rangle}{\sqrt{\langle (\delta j_{i\downarrow}^{+L})^2 \rangle}} \right] \\
&= \frac{(1-2\langle n_{i\downarrow} \rangle)}{4\langle (\delta n_{i\downarrow})^2 \rangle} \frac{1}{\tau} \left[\frac{\langle j_{i\downarrow}^{+R} \rangle}{\sqrt{\langle (\delta j_{i\downarrow}^{+R})^2 \rangle}} - \frac{\langle j_{i\downarrow}^{+L} \rangle}{\sqrt{\langle (\delta j_{i\downarrow}^{+L})^2 \rangle}} \right].
\end{aligned}$$

- [1] S. M. Cronenwett *et al.*, Phys. Rev. Lett. **88**, 226805 (2002).
- [2] L. DiCarlo *et al.*, Phys. Rev. Lett. **97**, 036810 (2006).
- [3] F. Sfigakis *et al.*, Phys. Rev. Lett. **100**, 026807 (2008).
- [4] S. Sarkozy *et al.*, Phys. Rev. B **79**, 161307(R) (2009).
- [5] S. M. Cronenwett, T. H. Oosterkamp, and L. P. Kouwenhoven, Science **281**, 540 (1998).
- [6] A. Kogan *et al.*, Phys. Rev. Lett. **93**, 166602 (2004).
- [7] S. Amasha, I. J. Gelfand, M. A. Kastner, and A. Kogan, Phys. Rev. B **72**, 045308 (2005).
- [8] T. S. Jespersen, M. Aagesen, C. Sorensen, P.E. Lindelof, and J. Nygard, Phys. Rev. B **74**, 233304 (2006).
- [9] V. Madhavan *et al.*, Science **280**, 567 (1998).
- [10] H. C. Manoharan, C. P. Lutz, and D. M. Eigler, Nature **403**, 512 (2000).
- [11] N. Néel *et al.*, Phys. Rev. Lett. **98**, 016801 (2007).
- [12] A. F. Otte *et al.*, Nat. Phys. **4**, 847 (2008).
- [13] Y. Meir and N. S. Wingreen, Phys. Rev. Lett. **68**, 2512 (1992).
- [14] S. Hershfield, J. H. Davies, and J. W. Wilkins, Phys. Rev. B **46**, 7046 (1992).
- [15] P. Fulde, *Electronic Correlations in Molecules and Solids* (Springer-Verlag, Berlin, 1993).
- [16] C. Lanczos, J. Res. Nat. Bur. Stand. **45**, 255 (1950).
- [17] E. Dagotto, Rev. Mod. Phys. **66**, 763 (1994).
- [18] H. Mori, Prog. Theor. Phys. **33**, 423 (1965).
- [19] R. Zwanzig, In *Lectures in Theoretical Physics* Vol. 3 (Interscience, New York, 1961).
- [20] J. Hong and W. Woo, Phys. Rev. Lett. **99**, 196801 (2007).
- [21] P. O. Löwdin, J. Math. Phys. **3**, 969 (1962).
- [22] V. Mujica, M. Kemp, and M. A. Ratner, J. Chem. Phys. **101**, 6849 (1994).
- [23] Y. Nagaoka, Phys. Rev. **138**, A1112 (1965).